Tetrahydrophthalic anhydride

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 3.79e-11 cm3/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 2.37e-01

Confidence level: 8.45e-01

Nearest Neighbors from the Training Set

Image not found
(3Z)-3-Hexenyl acetate
Measured: 7.80e-11
Predicted: 7.52e-11

Image not found
Cyclopropaneacetaldehyde, 2,2-dimethyl-3-(2-oxopropyl)-
Measured: 4.80e-11
Predicted: 4.73e-11

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alpha-Angelica lactone
Measured: 6.90e-11
Predicted: 6.33e-11

Image not found
Glutaraldehyde
Measured: 2.38e-11
Predicted: 2.50e-11

Image not found
Dimethyl adipate
Measured: 8.40e-12
Predicted: 6.84e-12